Coherent Hard X-ray Beamline

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BROOKHAVEN NATIONAL LABORATORY

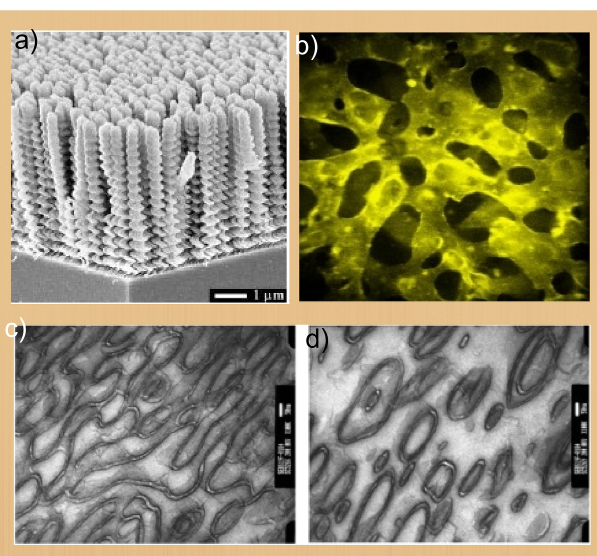
NATIONAL SYNCHROTRON LIGHT SOURCE II project beamlines • funded by DOE

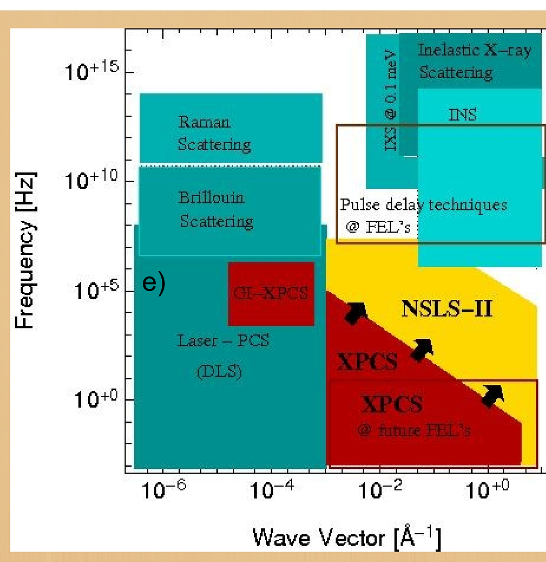
SCIENTIFIC MISSION

Studies of the interplay between nano-scale dynamics, structure and macroscopic properties in:

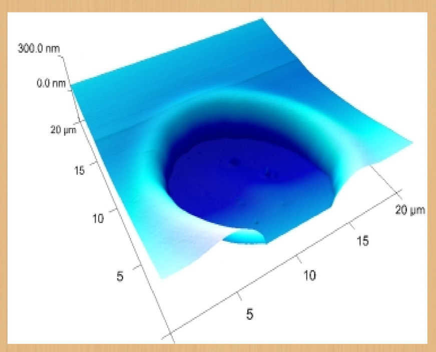
- •soft matter and biological materials e.g. complex fluids (polymers, colloidal glasses and gels, liquid crystals), liquid and polymer surfaces and interfaces, proteins in solution and crystals
- •driven and out of equilibrium systems e.g. complex fluids under flow/shear, structural phase transitions
- •heterogeneous systems e.g. time- and space-resolved dynamical heterogeneities
- •Inorganic materials e.g. metallic glasses, phase ordering crystals

"How do we characterize and control matter away- especially very far away- from equilibrium?"

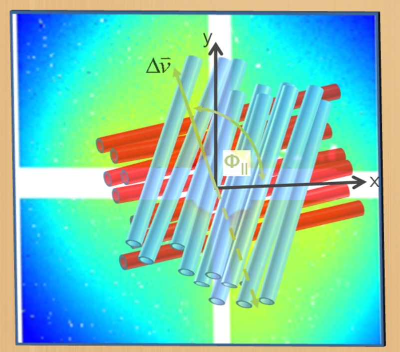




a-d Examples of microstructure: porous silicon (a); bicontinuous microstructure arrested by interfacial colloidal jamming (A. Moharaz) (b) sponge phase in a polymer blend (S. Mochrie) (c-d); e) phase space accessible today and at NSLS-II. The NSLS-II source will enable studies of dynamics on faster time scales and shorter length scales than is possible at current sources



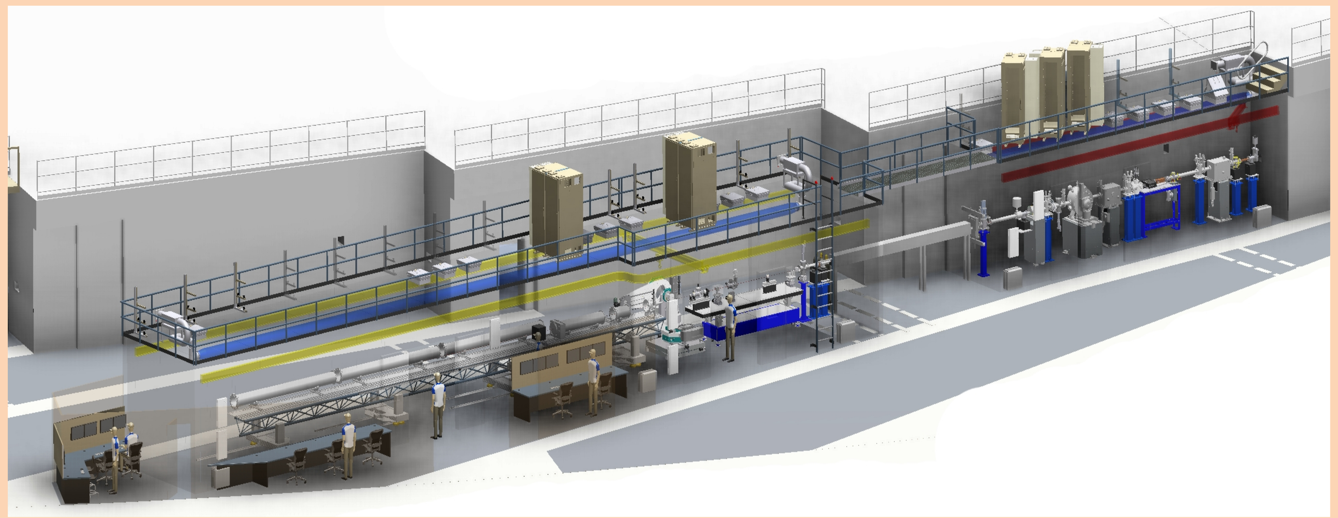
Dewetting dynamics from polymer interfaces
AF, L. Lurio, J. Lal, M. Sutton - P45.00003

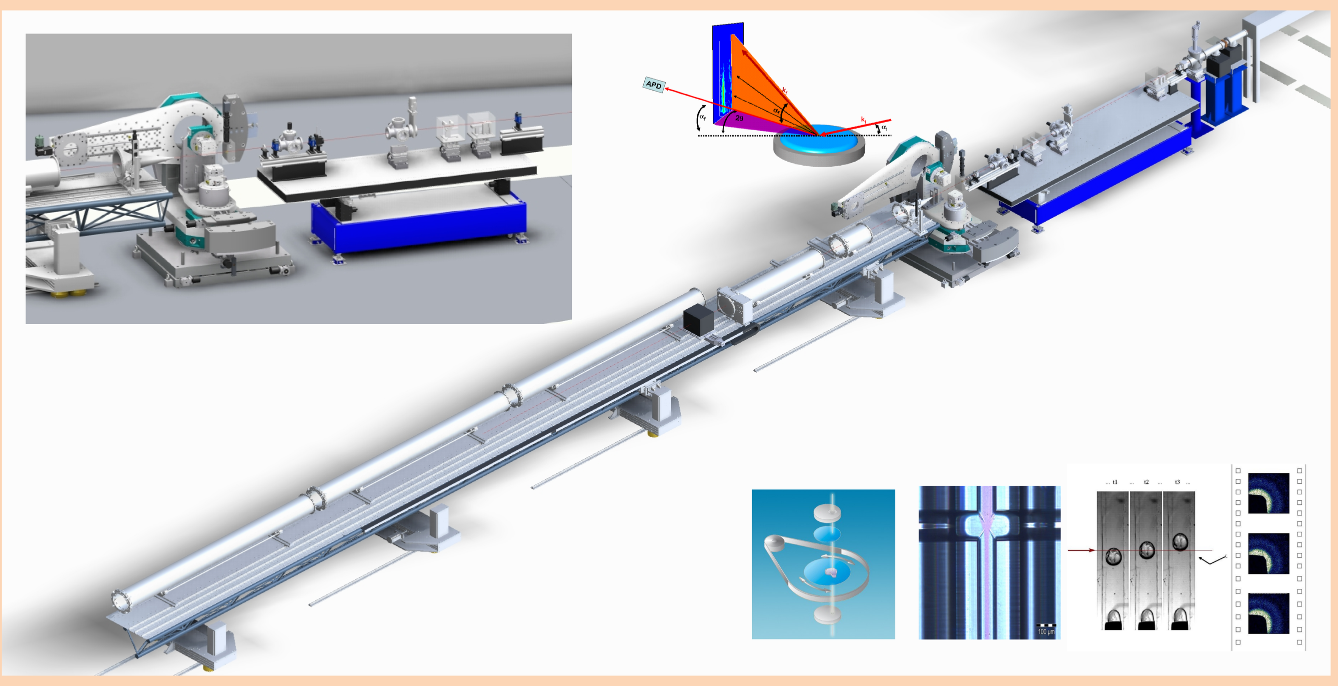


Self-assembling organic nanotubes
LW, P. Terrech, C. Caronna - Z47.00003

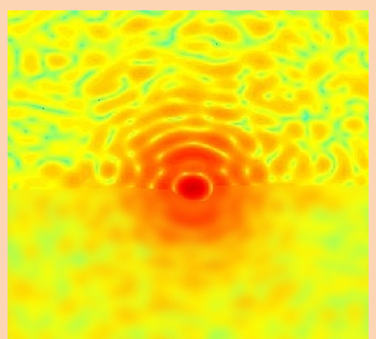
TECHNIQUES AND CAPABILITIES

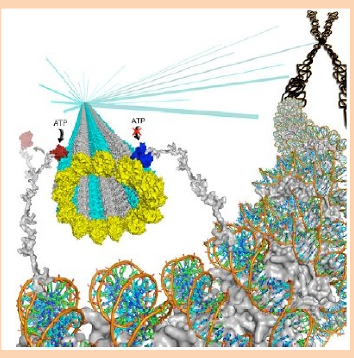
- •Studies of dynamics with *X-ray Photon Correlation Spectroscopy*
- •Signal-to-noise (SNR) in XPCS: *SNR~brightness x (time)*$^{1/2}$
- •Hence: a *10x increase* in brightness at NSLS-II will allow measurement of *100x faster fluctuations* with the same SNR
- •Coherent diffraction in SAXS, GI-SAXS, WAXS
- •Capabilities for Coherent Diffraction Imaging (CDI)
- •Consolidated Endstation instrument for small angle scattering
- •Sample environments: cryo-furnace for SAXS/WAXS; flow/shear-cell; Microfluidic chips; Langmuir trough for surface studies; scanning XRD microscope for ptycographic CDI, etc
- •Optical design optimized for very high mechanical stability and coherent wavefront preservation
- •Flexible focusing scheme using refractive optics
- •Spot size: ~10 µm for SAXS, ~1-2 µm for WAXS
- •Energy range: 6-16 keV,
- •Monochromatic ($\Delta\lambda/\lambda \sim 10^{-4}$) or pink ($\Delta\lambda/\lambda \sim 5\cdot 10^{-3}$) beam





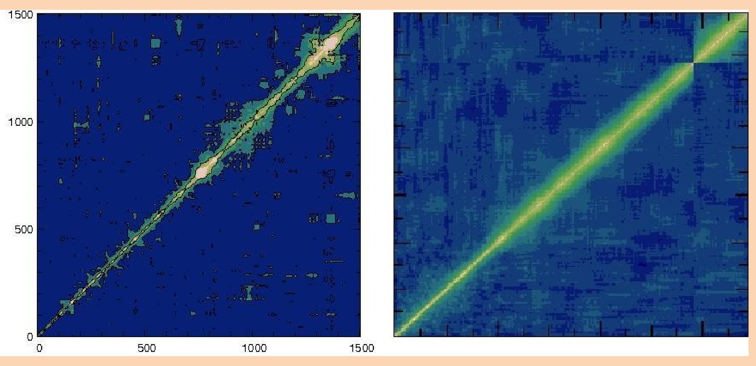
EXAMPLES of SCIENTIFIC OPPORTUNITIES





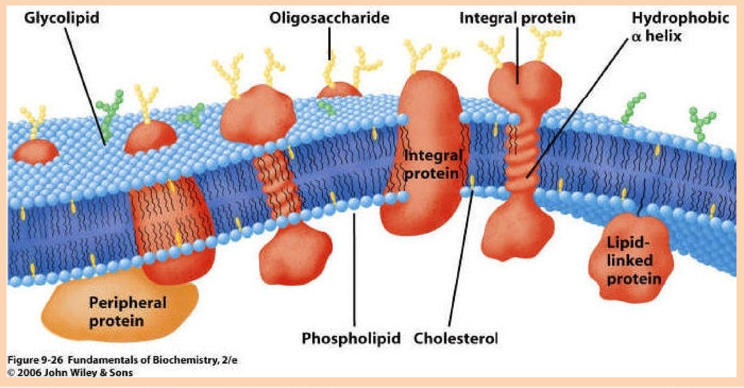
Speckle patterns (left) simulating a "blurring" effect that motion of proteins inside a crystal will create in diffuse coherent diffraction patterns. Motion of motor proteins (right: NOD structure, J. Cochran et al.) will be measured from the speckle visibility

Protein dynamics: Measuring the dynamics of proteins in a crystal can provide invaluable information in understanding their biological function. Molecular motion in protein microcrystals coupled over large scales generate diffraction spots (speckles) around the main Bragg peaks. Here we propose to measure (for the first time) dynamic information about this motion by analyzing the speckle contrast in coherent diffraction patterns.



Two-time correlation functions showing non-equilibrium effects ("aging") and heterogeneous dynamics (left) in colloidal gels or dynamical "rare events" in a colloidal glass (right)

Non-equilibrium dynamics and self-organization in soft-matter systems: studies of "Matter far beyond equilibrium" was recently identified as one of "Five challenges for science and imagination" in a report to the DOE by BESAC. The CHX instrument will be ideally adapted to address this challenge related to the DOE scientific program. The experiments will focus on understanding complex dynamics in non-equilibrium and driven (e.g. by flow/shear) soft matter systems and the interplay between molecular scale structure, mesoscale dynamics, and macroscopic properties such as the advective response to shear



Cartoon of a biomembrane. Characteristic length scales range from nanometers (the thickness of a biomembrane) to micrometers (the length of polymers that form the cytoskeleton). They are chemically diverse – building blocks include proteins, nucleic acids, lipids and polysaccharides – and formidably complex.

Non-equilibrium dynamics model and artificial membranes:
Goal: understand the relationship and interplay between structure, dynamics, and function.
Biomembrane visco-elasticity can both influence and be influenced by membrane protein conformation, leading potentially to elastically mediated interactions between proteins (Rheinstadter *et al.*, *Phys. Rev. Lett.* **103**, 128104 , 2004). Goal for XPCS: visco-elastic properties at length scales (10's of nm) matching typical protein-protein separations. Fluctuations of membrane lipid rafts that could also be measured by XPCS at NSLS-II could be used as "fingerprints" to distinguish between different scenarios proposed for the raft formation
(J. Fan, M. Haataja *et al.*, *Phys. Rev. Lett.* **104**, 118101, 2010).